Octane

111-65-9 | DTXSID0026882

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.62

Global applicability domain: Inside

Local applicability domain index: 9.96e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

Image not found
Octane
Measured: 3.35
Predicted: 3.62

Image not found
Chlorobenzene
Measured: 3.31
Predicted: 3.63

Image not found
Anisole
Measured: 4.01
Predicted: 3.76

Image not found
Pentyl acetate
Measured: 4.12
Predicted: 3.95

Image not found
Propane, 1,1'-oxybis[2-methyl-
Measured: 3.40
Predicted: 3.47